

A Study on Shape of Te Isotopes in Mean Field Formalism

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Abstract. The systematic investigation of ground-state shape evolution from γ -unstable O(6) to spherical U(5) for even-even $^{112-134}\text{Te}$ has been presented by using the quadrupole moment constrained Hartree-Fock-Bogoliubov (HFB) method with the Skyrme force SLy4. ^{124}Te has been pointed out as to be the possible critical-point nucleus with E(5) symmetry.

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1. Introduction

Spherical vibrator, rotational ellipsoid, and deformed shapes of nuclei are related with modes of collective motion and geometric shapes of nuclei [1, 2, 3, 4]. When the number of protons and neutrons is changed, nuclei can show changes of their energy levels and electromagnetic transition rates among collective modes of nuclei. Transitions from one kind of collective behavior to another are named shape phase transition. These transitions are quantum phase transitions (QPTs) [5]. They are different from thermal phase transitions which occur as a function of temperature. This implies changes in the shape of the nucleus. The control parameter is the number of nucleons. In the last decade, many researchers have given insights into the evolution of structure of nuclei (in particular transitional regions of rapid change) [6]. They have used the concepts of QPTs, phase coexistence and the critical-point symmetries (CPS) [7, 8] proposed by Iachello, as well as a raft of geometrical models [9, 10, 11, 12, 13, 14].

Theoretically, QPTs have been mostly studied in the Interacting Boson Model (IBM). It holds the $U(5)$, $SU(3)$ and $O(6)$ symmetries within the simplest $U(6)$ symmetry. The $U(5)$, $SU(3)$ and $O(6)$ dynamical symmetries correspond to the shape phase of a spheroid, axially prolate rotor and γ -soft rotor, respectively [15]. Using the model, the authors pointed out that second order shape phase transition occurs between $U(5)$ and $O(6)$ while first order shape phase transition occurs between $O(6)$ and $SU(3)$ [16, 17]. More recently, Iachello has pointed out that the properties of nuclei lying at the critical-point of a shape phase transition can be described by special solutions of the Bohr Hamiltonian, called as critical-point symmetries. The $E(5)$ critical-point symmetry [7] corresponds to the second order critical-point between $U(5)$ and $O(6)$, while the $X(5)$ critical-point symmetry [8] corresponds to the first order transition between $U(5)$ and $SU(3)$. Experimentally, The $E(5)$ and $X(5)$ symmetry has been realized in the spectrum of ^{134}Ba [18] and ^{152}Sm [19], respectively. The introduction of critical-point symmetries $E(5)$ and $X(5)$, and their experimental realizations have triggered many works on quantum phase transitions [20].

In spite of the fact that the IBM and the solutions of Bohr Hamiltonian are useful for determining shape phase transitions in nuclei, mean field formalisms (e.g., HFB method [2, 21, 22] and relativistic mean field (RMF) model [23, 24, 25, 26]) which provide a correct prediction of many nuclear phenomena have been successfully used to study the shape phase transition in nuclei. The RMF theory has been used to investigate the critical-point nuclei in even-even Sm [27] and Ce [28] isotopes. In these studies, $^{148,150,152}\text{Sm}$ and $^{128,130,132,134}\text{Ce}$ have been suggested as an example of the possible critical-point nuclei with $X(5)$ symmetry. Beside, Ti isotopes have been examined in the HFB method [29] and RMF model [30] to investigate the critical-point nuclei. In these studies, $^{48,52,60}\text{Ti}$ and $^{46,52,60}\text{Ti}$ have been found as to be the possible candidate critical-point nuclei with $E(5)$ symmetry in the RMF model and HFB method,

respectively. A series of isotopes in rare-earth region have been found as to be possible critical-point nuclei [31, 32]. Also, Mo isotopes were investigated by using the RMF theory [33, 34] and ^{94}Mo has been suggested as to be γ -unstable nucleus in Ref. [33]. In these studies, potential energy curves (PECs) come by quadrupole moment constrained calculations have been examined in order to identifying of the critical-point nuclei. Relatively flat PECs correspond to the critical-point nuclei with E(5) symmetry, while PECs with a bump correspond to the X(5) symmetry (The relation between shape phase transition and PECs can be found in [6, 35]). However, for a quantitative analysis of QPTs in nuclei electromagnetic transition rates and ratios of excitation energies should be calculated [36]. For this reason, the generator coordinate method (GCM) has been used to perform configuration mixing of angular-momentum and particle-number projected relativistic wave functions restricted to axial symmetry in [37]. In recent years, the GCM has been extended on triaxial states [38, 39, 40]. Nevertheless, the application of these methods in a systematic study of shape transition is at present still very time-consuming because of its triaxiality. It should be noted, however, that the potential energy curves obtained from quadrupole moment constrained calculations are important, and can provide a qualitative understanding of the shape phase transition. Particularly, the evolution of the PECs along the isotopic or isotonic chains can be useful for investigation of shape phase transitions in nuclei.

Rapid shape changes in nuclei have been known for about half a century [6]. Classic shape transition regions take place in the light Si-Mg region [41], near $A = 100$ ($Z \sim 40$) [42], light rare-earth region ($A \sim 150$) and actinides. Beside, the γ -unstable character of nuclei in the mass region $A = 120 - 130$ was pointed out in [43] many years ago. And, ^{124}Te in this region was experimentally investigated and suggested to be a possible γ -soft nucleus [44]. In this study, constrained HFB method has been used to obtain the ground-state properties of even-even $^{112-134}\text{Te}$ isotopes such as total binding energy and quadrupole deformation. The shape evolution of Te isotopes has been analyzed by examining their PECs.

2. The theoretical framework and numerical details

In the HFB formalism, a two-body Hamiltonian of a system of fermions by means of a set of annihilation and creation operators (c , c^\dagger) is given by

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c_{n_1}^\dagger c_{n_2} + \frac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c_{n_1}^\dagger c_{n_2}^\dagger c_{n_4} c_{n_3}, \quad (1)$$

where $\bar{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$ are anti-symmetrized matrix elements of the two-body N-N interaction. The ground-state wave function $|\Phi\rangle$ is described as the quasi-particle vacuum $\alpha_k |\Phi\rangle = 0$ and the linear Bogoliubov transformation:

$$\alpha_k = \sum_n (U_{nk}^* c_n + V_{nk}^* c_n^\dagger), \quad \alpha_k^\dagger = \sum_n (V_{nk} c_n + U_{nk} c_n^\dagger) \quad (2)$$

provides connection between the quasiparticle operators (α, α^\dagger) and the original particle operators. The basic building blocks of the theory are the density matrix and the pairing tensor. In terms of the normal ρ and pairing κ one-body density matrices:

$$\rho_{nn'} = \langle \Phi | c_{n'}^\dagger c_n | \Phi \rangle = (V^* V^T)_{nn'}, \quad \kappa_{nn'} = \langle \Phi | c_{n'} c_n | \Phi \rangle = (V^* U^T)_{nn'}, \quad (3)$$

the expectation value of the Hamiltonian (1) could be expressed in terms of an energy functional:

$$E[\rho, \kappa] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \text{Tr}[(e + \frac{1}{2}\Gamma)\rho] - \frac{1}{2}\text{Tr}[\Delta\kappa^*] \quad (4)$$

where $\Gamma_{n_1 n_3} = \sum_{n_2 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2}$ and $\Delta_{n_1 n_2} = \frac{1}{2} \sum_{n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}$. Modern energy functional (4) includes terms that cannot be simply related to some prescribed effective interaction [45]. In terms of Skyrme forces, the HFB energy (4) has the form of local energy density functional:

$$E[\rho, \tilde{\rho}] = \int d^3\mathbf{r} H(\mathbf{r}), \quad (5)$$

where $H(\mathbf{r}) = H(\mathbf{r}) + \tilde{H}(\mathbf{r})$ is the sum of the mean field and pairing energy densities. The variation of the energy (5) according to the particle local density ρ and pairing local density $\tilde{\rho}$ results in Skyrme HFB equations:

$$\begin{aligned} & \sum_{\sigma'} \begin{pmatrix} h(\mathbf{r}, \sigma, \sigma') & \tilde{h}(\mathbf{r}, \sigma, \sigma') \\ \tilde{h}(\mathbf{r}, \sigma, \sigma') & -h(\mathbf{r}, \sigma, \sigma') \end{pmatrix} \begin{pmatrix} U(E, \mathbf{r}\sigma') \\ V(E, \mathbf{r}\sigma') \end{pmatrix} \\ &= \begin{pmatrix} E + \lambda & 0 \\ 0 & E - \lambda \end{pmatrix} \begin{pmatrix} U(E, \mathbf{r}\sigma) \\ V(E, \mathbf{r}\sigma) \end{pmatrix}, \end{aligned} \quad (6)$$

where λ is chemical potential. Local fields $h(\mathbf{r}, \sigma, \sigma')$ and $\tilde{h}(\mathbf{r}, \sigma, \sigma')$ can be calculated in the coordinate space [2, 46].

The HFB equations (5) have been solved by expanding quasi-particle wave functions that conserve axial symmetry and parity on a harmonic oscillator basis expressed in coordinate space prescribed by Stoitsov *et al.* [46] in the present study. For pairing, the zero-range pairing interaction is taken into account and Lipkin-Nogami method is employed (Further details are given in Ref. [46]). The oscillator parameter b_0 is chosen as to be $b_0 = \sqrt{2(\hbar^2/2m)(49.2A^{-1/3})}$. In order to obtain the potential energy curves (PECs) in the present study, the standard quadratic form of the quadrupole constraint [21, 46] has been performed. The standard quadratic form can be interpreted by the formula $E^Q = C_Q(\langle \hat{Q} \rangle - \bar{Q})^2$, where C_Q is the stiffness constant, $\langle \hat{Q} \rangle$ is the average value of the mass quadrupole moment operator ($\hat{Q} = 2z^2 - r^2$) and \bar{Q} is the constraint value of the quadrupole moment. For describing the deformation of nuclei, the quadrupole deformation parameter is commonly used rather than quadrupole moments. The relation between the constraint quadrupole moment \bar{Q} and constraint quadrupole deformation parameter $\bar{\beta}_2$ is given by the formula $\bar{\beta}_2 = \sqrt{\pi/5} \langle \bar{Q} \rangle / \langle r^2 \rangle$ [46]. 16 oscillator shells have been taken into account in the present calculations. There can be found

a number of effective Skyrme forces in literature for correct prediction of the nuclear ground-state properties of nuclei [47, 48, 49]. In this work, the Skyrme force SLy4 [49] has been used to calculate ground-state properties of even–even Te isotopes with $60 \leq N \leq 82$.

3. Results and discussions

The calculated total binding energies for even–even $^{112-134}\text{Te}$ isotopes obtained from the constrained HFB method with the SLy4 parameter set are tabulated in Table 1. Also, the predictions of RMF model [50] and the experimental data [51] are listed for comparison. The total binding energies of all isotopes are reproduced well by the SLy4 Skyrme force. The deviations are at most 0.3%. Also, as can be seen in Table 1, the predictions of RMF model with NL3 interaction are in a good agreement with the experimental data. The mean differences between experimental data and the predictions of the HFB method and RMF model with NL3 interaction are 2.532 and 1.688 MeV, respectively. For this reason, it can be pointed out that the predictions of both HFB method and RMF model are good in describing the ground-state binding energies of $^{112-134}\text{Te}$.

The mean field formalism based on the Hartree-Fock approximation with phenomenological effective interactions is important in the microscopic description of nuclei [52, 53]. It allows a unified description of the ground-state properties for nuclei throughout the nucleidic chart. One of the great achievement of the theory is that not only it can reproduce binding energies and densities, but it also provides a good description of the size of the ground-state deformations in nuclei [54]. In this study, the quadrupole deformation parameters β_2 for $^{112-134}\text{Te}$ have been obtained from constrained HFB method with SLy4 Skyrme force. They are shown in Fig. 1. Also, the predictions of RMF model with NL3 interaction [50] and the experimental data [55] are shown for comparison. As can be seen in the Fig. 1, the calculated β_2 values obtained from HFB method with SLy4 parameters are in good agreement with the experimental data. Only amplitude of quadrupole deformation parameter β_2 values obtained from both of the HFB method and RMF model are given in the Fig. 1 and the exact values of β_2 are listed in Table 2. It should be noted, however, that β_2 cannot be observed directly from an experiment. To obtain the β_2 value from an experiment, a conventional way is that the electric quadrupole transition rate from ground-state 0^+ to the 2^+ state $B(E2) \uparrow$ can be used [55]. The correlation between $B(E2) \uparrow$ and β_2 is given by the formula $\beta_2 = (4\pi/3ZR_0^2)[B(E2) \uparrow / e^2]^{1/2}$ where $R_0 = 1.2A^{1/3}$. The formula based on rigid rotor cannot always represent a parameter of deformation. The extracting of β_2 is questionable in the case of spherical nuclei, because $B(E2) \uparrow$ connects vibrational states in the spherical nuclei. In particular, the radius R_0 is so small for light nuclei. This elicits a very large β_2 deformation with the formula. However, in medium-mass and heavy region usage of the formula is suitable [30].

In this study, the constrained HFB method with Skyrme force SLy4 is employed for the investigation of shape evolution of even–even $^{112-134}\text{Te}$ because of its success in describing the binding energies and quadrupole deformation parameters for Te isotopes. In Fig. 2, the potential energy curves (PECs) for $^{112-134}\text{Te}$. In the figure, the total binding energy of Te isotopes for the ground-state is taken as to be the reference. In the Fig. 2, starting from ^{112}Te to ^{120}Te , the nuclei have oblate shape. In the PECs of the $^{122-126}\text{Te}$, their barriers against deformation are weak which means that these nuclei may be in a transitional region. In particular, the PEC of ^{124}Te in the Fig. 2 seems flat from $\beta_2 = -0.2$ to $\beta_2 = 0.25$. Through these β_2 ranges, the variation of the binding energies in the PEC of ^{124}Te are less than 0.4 MeV. This implies that the barriers against deformation are very weak, and ^{124}Te maybe a possible example of the critical-point nuclei with E(5) symmetry. With increasing of neutron numbers starting from the ^{128}Te to ^{132}Te , shape of Te isotopes have become prolate and finally ^{134}Te which has shell closure with magic neutron numbers $N = 82$ are found to be as spherical.

In Table 3, the differences of the binding energy between the spherical-state and the ground-state of even-even $^{112-134}\text{Te}$ isotopes are shown to understanding of how the shape of the Te isotopes changes with the neutron number as an additional evidence to the results of the PECs. They can show how soft the nucleus is against deformation. The calculated binding energy differences between the spherical-state and the ground-state of $^{112-134}\text{Te}$ isotopes changes from 0 to 2.572 MeV. Drastic changes are clearly visible around $^{120-124}\text{Te}$ in the binding energy differences. There is a clear jump appearing at ^{124}Te which implies that ^{124}Te can be a possible candidate critical-point nuclei with E(5) symmetry.

As an additional evidence for confirmation of the result of this study, the ratios of experimental excitation energies of ^{124}Te nucleus [44] are given in Table 4. Also, the U(5), X(5), SU(3), E(5) and O(6) symmetry predictions are listed for comparison [7, 8, 44]. The characteristic ratio $R_{4/2} = E(4_1^+)/E(2_1^+)$ and the ratio of the energies of the first two excited 0^+ states $R_{0/2} = E(0_2^+)/E(2_1^+)$ are tabulated. As can be seen in Table 4, the E(5) symmetry values obtained from solution of Bohr-Mottelson differential equations for $R_{4/2}$ and $R_{0/2}$ is 2.20 and 3.03, respectively. They are closer to the observed ratios $R_{4/2} = 2.07$ and $R_{0/2} = 2.75$ which means that ^{124}Te may hold the E(5) symmetry.

4. Summary

The total binding energies and quadrupole deformation parameters for even–even $^{112-134}\text{Te}$ isotopes have been calculated in the constrained HFB method with Skyrme SLy4 force as in a good agreement with experimental data. The ground-state shape evolution of these nuclei are investigated by using the potential energy curves. ^{124}Te

has been found as to be an example for possible critical-point nucleus, which marks the phase transition between spherical $U(5)$ and γ -unstable shapes $O(6)$. It should be noted, however, that this work investigates only the PECs of Te isotopes with respect to the β degree of freedom. For a quantitative identifying of the $E(5)$ symmetry in Te isotopes, one should go beyond mean field.

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Table 1. The total binding energy for the ground-state of $^{112-134}\text{Te}$ in units of MeV.

| | This work | RMF [50] | Exp [51] |
|-------------------|-----------|----------|----------|
| ^{112}Te | 937.821 | 938.880 | 940.610 |
| ^{114}Te | 958.058 | 959.060 | 961.337 |
| ^{116}Te | 977.630 | 978.530 | 980.860 |
| ^{118}Te | 996.680 | 997.600 | 999.454 |
| ^{120}Te | 1014.148 | 1015.640 | 1017.281 |
| ^{122}Te | 1030.893 | 1032.530 | 1034.333 |
| ^{124}Te | 1047.472 | 1049.160 | 1050.686 |
| ^{126}Te | 1063.296 | 1066.980 | 1066.368 |
| ^{128}Te | 1078.858 | 1080.750 | 1081.439 |
| ^{130}Te | 1094.204 | 1096.430 | 1095.941 |
| ^{132}Te | 1108.850 | 1112.220 | 1109.914 |
| ^{134}Te | 1123.508 | 1126.430 | 1123.435 |

Table 2. The ground-state quadrupole deformation parameter β_2 for Te isotopes.

| | This work | RMF [50] | Exp [51] |
|-------------------|-----------|----------|----------|
| ^{112}Te | 0.187 | 0.164 | |
| ^{114}Te | 0.304 | 0.232 | |
| ^{116}Te | -0.171 | 0.257 | |
| ^{118}Te | -0.173 | 0.175 | |
| ^{120}Te | -0.169 | 0.179 | 0.201 |
| ^{122}Te | -0.135 | 0.161 | 0.185 |
| ^{124}Te | -0.096 | 0.138 | 0.170 |
| ^{126}Te | -0.093 | -0.003 | 0.153 |
| ^{128}Te | 0.076 | -0.002 | 0.136 |
| ^{130}Te | 0.062 | 0.032 | 0.118 |
| ^{132}Te | 0.028 | 0.000 | |
| ^{134}Te | -0.005 | 0.000 | |

Table 3. The difference of the total binding energy (in units of MeV) between the spherical state and the ground-state of $^{112-134}\text{Te}$ obtained by the constrained HFB method with SLy4 Skyrme force.

| Nuclei | HFB-SLy4 |
|-------------------|----------|
| ^{112}Te | 2.329 |
| ^{114}Te | 2.397 |
| ^{116}Te | 2.519 |
| ^{118}Te | 2.572 |
| ^{120}Te | 1.900 |
| ^{122}Te | 1.259 |
| ^{124}Te | 0.354 |
| ^{126}Te | 0.410 |
| ^{128}Te | 0.227 |
| ^{130}Te | 0.160 |
| ^{132}Te | 0.053 |
| ^{134}Te | 0.000 |

Table 4. The ratios of available experimental excitation energies for ^{124}Te isotopes with some theoretical predictions for comparison [6–8, 44].

| | $R_{4/2}$ | $R_{0/2}$ |
|-------|-----------|-----------|
| U(5) | 2.00 | 2.00 |
| X(5) | 2.91 | 5.67 |
| SU(3) | 3.33 | $\gg 2$ |
| E(5) | 2.20 | 3.03 |
| O(6) | 2.50 | 4.50 |
| Exp | 2.07 | 2.75 |

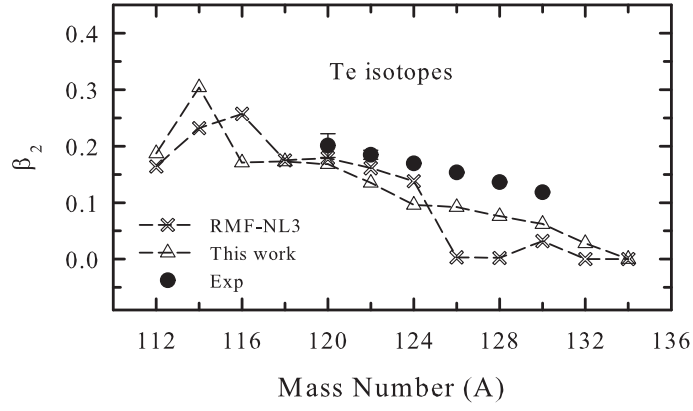


Figure 1. The ground-state quadrupole deformation parameter for Te isotopes. The predictions of the HFB method with SLy4 Skyrme force are compared with the those of the RMF model with NL3 interaction and experimental results.

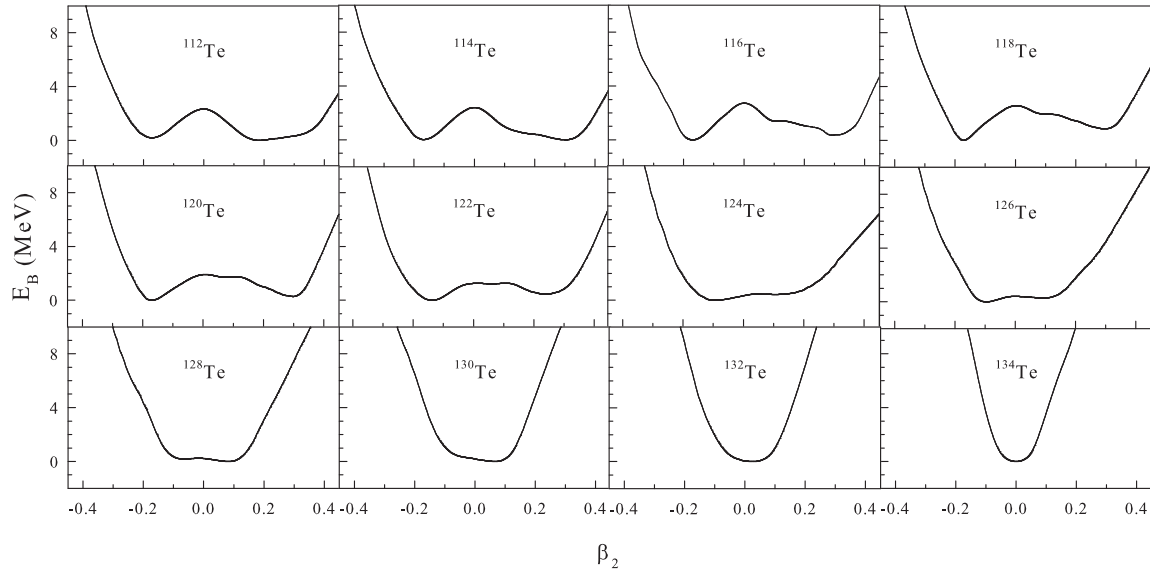


Figure 2. The potential energy curves for $^{112-134}\text{Te}$ obtained from the constrained HFB method with SLy4 Skyrme force.